10521799.trn

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PASSWORD:
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NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	DEC 18	CA/CAplus pre-1967 chemical substance index entries enhanced with preparation role
NEWS 4	DEC 18	CA/CAplus patent kind codes updated
NEWS 5	DEC 18	MARPAT to CA/CAplus accession number crossover limit increased to 50,000
NEWS 6	DEC 18	MEDLINE updated in preparation for 2007 reload
NEWS 7	DEC 27	CA/CAplus enhanced with more pre-1907 records
NEWS 8	JAN 08	CHEMLIST enhanced with New Zealand Inventory of Chemicals
NEWS 9	JAN 16	CA/CAplus Company Name Thesaurus enhanced and reloaded
NEWS 10	JAN 16	IPC version 2007.01 thesaurus available on STN
NEWS 11	JAN 16	WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
NEWS 12	JAN 22	CA/CAplus updated with revised CAS roles
NEWS 13	JAN 22	CA/CAplus enhanced with patent applications from India
NEWS 14	JAN 29	PHAR reloaded with new search and display fields
NEWS 15	JAN 29	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS 16	FEB 15	PATDPASPC enhanced with Drug Approval numbers
NEWS 17	FEB 15	RUSSIAPAT enhanced with pre-1994 records
NEWS 18	FEB 23	KOREAPAT enhanced with IPC 8 features and functionality
NEWS 19	FEB 26	MEDLINE reloaded with enhancements
NEWS 20	FEB 26	EMBASE enhanced with Clinical Trial Number field
NEWS 21	FEB 26	TOXCENTER enhanced with reloaded MEDLINE
NEWS 22	FEB 26	IFICDB/IFIPAT/IFIUDB reloaded with enhancements
NEWS 23	FEB 26	CAS Registry Number crossover limit increased from 10,000 to 300,000 in multiple databases
NEWS 24	MAR 15	WPIDS/WPIX enhanced with new FRAGHITSTR display format
NEWS 25	MAR 16	CASREACT coverage extended
NEWS 26	MAR 20	MARPAT now updated daily
NEWS 27	MAR 22	LWPI reloaded
NEWS 28	MAR 30	RDISCLOSURE reloaded with enhancements
NEWS 29	MAR 30	INPADOCDB will replace INPADOC on STN
NEWS 30	APR 02	JICST-EPLUS removed from database clusters and STN

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8
NEWS X25	X.25 communication option no longer available

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Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 07:16:33 ON 15 APR 2007

=>
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THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE
Do you want to switch to the Registry File?
Choice (Y/n):
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Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 07:16:45 ON 15 APR 2007
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 13 APR 2007 HIGHEST RN 930268-90-9
DICTIONARY FILE UPDATES: 13 APR 2007 HIGHEST RN 930268-90-9

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TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

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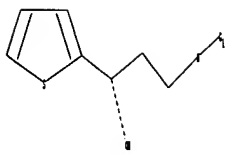
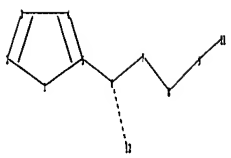
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10521799.str





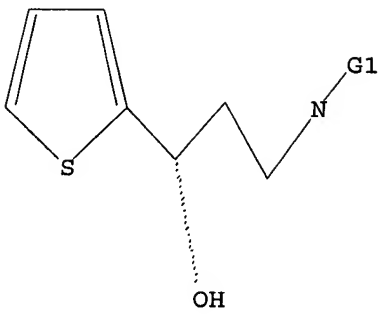
chain nodes :
6 7 8 9 11 12
ring nodes :
1 2 3 4 5
chain bonds :
5-6 6-7 6-12 7-8 8-9 9-11
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
6-12 8-9 9-11
exact bonds :
1-2 1-5 2-3 3-4 4-5 5-6 6-7 7-8
isolated ring systems :
containing 1 :

G1:H,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
11:CLASS 12:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 H,Ak

Structure attributes must be viewed using STN Express query preparation.

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=> s l1
SAMPLE SEARCH INITIATED 07:19:12 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      453 TO ITERATE

100.0% PROCESSED      453 ITERATIONS                          15 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          7784 TO    10336
PROJECTED ANSWERS:               68 TO      532

L2            15 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 07:19:18 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     9242 TO ITERATE

100.0% PROCESSED     9242 ITERATIONS                         328 ANSWERS
SEARCH TIME: 00.00.01

L3           328 SEA SSS FUL L1

=> FIL HCAPLUS
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                             173.90     174.11

FILE 'HCAPLUS' ENTERED AT 07:19:36 ON 15 APR 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 15 Apr 2007 VOL 146 ISS 17
FILE LAST UPDATED: 13 Apr 2007 (20070413/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

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=> s l3
L4          188 L3

=> s l4 and process
       2409591 PROCESS
       1638936 PROCESSES
       3596091 PROCESS
                 (PROCESS OR PROCESSES)
L5           38 L4 AND PROCESS

=> s l5 and enantiomer
         23897 ENANTIOMER
         27436 ENANTIOMERS
         39311 ENANTIOMER
                 (ENANTIOMER OR ENANTIOMERS)
L6            4 L5 AND ENANTIOMER

=> s l5 and enantiomer-enriched
         23897 ENANTIOMER
         27436 ENANTIOMERS
         39311 ENANTIOMER
                 (ENANTIOMER OR ENANTIOMERS)
        128305 ENRICHED
             1 ENRICHEDS
        128306 ENRICHED
                 (ENRICHED OR ENRICHEDS)
            54 ENANTIOMER-ENRICHED
                 (ENANTIOMER(W)ENRICHED)
L7            0 L5 AND ENANTIOMER-ENRICHED

=> s l5 and catalyst
        759789 CATALYST
        757482 CATALYSTS
        970541 CATALYST
                 (CATALYST OR CATALYSTS)
L8           15 L5 AND CATALYST

=> s l8 and bidentate
         23787 BIDENTATE
           128 BIDENTATES
         23865 BIDENTATE
                 (BIDENTATE OR BIDENTATES)
L9            3 L8 AND BIDENTATE

=> s l8 and bidentate phosphorus
         23787 BIDENTATE
           128 BIDENTATES
         23865 BIDENTATE
                 (BIDENTATE OR BIDENTATES)
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        313451 PHOSPHORUS
             1 PHOSPHORUSES
             2 PHOSPHORI
             8 PHOSPHORIS
        313460 PHOSPHORUS
                  (PHOSPHORUS OR PHOSPHORUSES OR PHOSPHORI OR PHOSPHORIS)
           111 BIDENTATE PHOSPHORUS
                  (BIDENTATE(W)PHOSPHORUS)
L10          0 L8 AND BIDENTATE PHOSPHORUS

=> s l8 and enantiomer-enriched
         23897 ENANTIOMER
         27436 ENANTIOMERS
         39311 ENANTIOMER
                  (ENANTIOMER OR ENANTIOMERS)
        128305 ENRICHED
             1 ENRICHEDS
        128306 ENRICHED
                  (ENRICHED OR ENRICHEDS)
            54 ENANTIOMER-ENRICHED
                  (ENANTIOMER(W)ENRICHED)
L11          0 L8 AND ENANTIOMER-ENRICHED

=> s l8 and enantiomer
         23897 ENANTIOMER
         27436 ENANTIOMERS
         39311 ENANTIOMER
                  (ENANTIOMER OR ENANTIOMERS)
L12          3 L8 AND ENANTIOMER

=> d his

     (FILE 'HOME' ENTERED AT 07:16:33 ON 15 APR 2007)

     FILE 'REGISTRY' ENTERED AT 07:16:45 ON 15 APR 2007
L1               STRUCTURE UPLOADED
L2            15 S L1
L3           328 S L1 SSS FULL

     FILE 'HCAPLUS' ENTERED AT 07:19:36 ON 15 APR 2007
L4           188 S L3
L5            38 S L4 AND PROCESS
L6             4 S L5 AND ENANTIOMER
L7             0 S L5 AND ENANTIOMER-ENRICHED
L8            15 S L5 AND CATALYST
L9             3 S L8 AND BIDENTATE
L10            0 S L8 AND BIDENTATE PHOSPHORUS
L11            0 S L8 AND ENANTIOMER-ENRICHED
L12            3 S L8 AND ENANTIOMER

=> d l6 ibib abs hitstr tot

L6   ANSWER 1 OF 4  HCAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:         2004:101154  HCAPLUS
DOCUMENT NUMBER:          140:163699
TITLE:                    Process for the preparation of
                          3-hydroxy-(2-thienyl)propanamines by catalytic
                          enantioselective hydrogenation of the corresponding
                          ketones
INVENTOR(S):              Hems, William; Rossen, Kai; Reichert, Dietmar;
```

Koehler, Klaus; Almena Perea, Juan Jose
PATENT ASSIGNEE(S): Degussa A.-G., Germany
SOURCE: PCT Int. Appl., 27 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004011452	A1	20040205	WO 2003-EP7927	20030721
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10233724	A1	20040205	DE 2002-10233724	20020724
DE 10258098	A1	20040701	DE 2002-10258098	20021211
CA 2493228	A1	20040205	CA 2003-2493228	20030721
AU 2003258532	A1	20040216	AU 2003-258532	20030721
EP 1523479	A1	20050420	EP 2003-771063	20030721
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1671685	A	20050921	CN 2003-817590	20030721
JP 2006502996	T	20060126	JP 2004-523756	20030721
US 2005272930	A1	20051208	US 2005-521799	20050121
IN 2005KN00259	A	20070105	IN 2005-KN259	20050224

PRIORITY APPLN. INFO.:

DE 2002-10233724	A	20020724
DE 2002-10258098	A	20021211
WO 2003-EP7927	W	20030721

OTHER SOURCE(S): CASREACT 140:163699; MARPAT 140:163699
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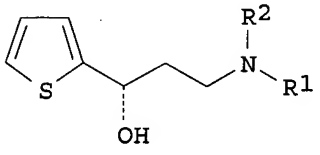

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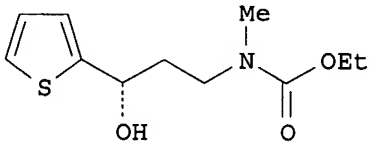


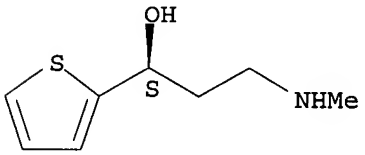
II

AB Title compds. I [wherein R1 and R2 = independently H, (cyclo)alkyl, acyl, alkoxycarbonyl, (hetero)aryl, (hetero)aralkyl, alkylcycloalkyl, alkyl(hetero)aryl; or NR1R2 = (un)substituted heterocyclyl], intermediates for the synthesis of enantiomer-pure bioactive substances, were prepared by catalytic enantioselective hydrogenation of the corresponding α-heteroaryl ketones. Inter alia Ru catalysts with chiral diamine and chiral biphosphine ligands were used. For example, 3-[N-ethoxycarbonyl-N-methylamino]-1-(2-thienyl)-1-propanone was introduced to a Buchi stirred autoclave, which was then evacuated. A mixture of (R)-TolBINAP-RuCl2-(1R,2R)-diphenylethylenediamine and KOBu-t in iPrOH was added. Flushing with H2, pressurizing to 10 bar, and heating to 40° for 2 h provided II in >96% yield with an enantiomeric excess

of 80.1%. The content of cyclic carbamate byproduct increased significantly after standing for a fairly long time.

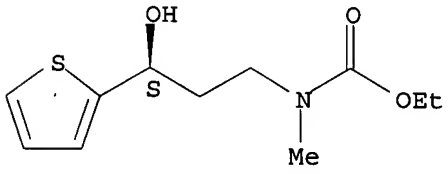
IT 116539-55-0P
RL: IMF (Industrial manufacture); PREP (Preparation)
(preparation of 3-hydroxy-(2-thienyl)propanamines by catalytic enantioselective hydrogenation of corresponding ketones)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT 586968-34-5P, (S)-3-[N-(Ethoxycarbonyl)-N-methylamino]-1-(2-thienyl)-1-propanol
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 3-hydroxy-(2-thienyl)propanamines by catalytic enantioselective hydrogenation of corresponding ketones)
RN 586968-34-5 HCAPLUS
CN Carbamic acid, [(3S)-3-hydroxy-3-(2-thienyl)propyl]methyl-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



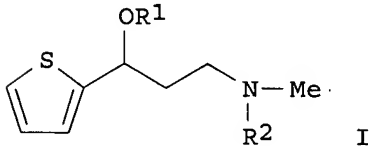
REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:931354 HCAPLUS
DOCUMENT NUMBER: 139:395802
TITLE: Preparation of propanolamine derivatives, process for preparation of 3-N-methylamino-1-(2-thienyl)-1-propanols, and process for preparation of propanolamine derivatives
INVENTOR(S): Inoue, Yoshiki; Mori, Hiroyuki; Nogami, Hiroyuki; Saitou, Takayuki; Ogura, Kuniyoshi
PATENT ASSIGNEE(S): Mitsubishi Rayon Co., Ltd., Japan
SOURCE: PCT Int. Appl., 98 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2003097632	A1	20031127	WO 2003-JP6225		20030519
W: CN, JP, US					
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR					
EP 1506965	A1	20050216	EP 2003-752916		20030519
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK					
US 2006167278	A1	20060727	US 2005-513790		20050527
PRIORITY APPLN. INFO.:			JP 2002-145394	A	20020520
			JP 2001-256621	A	20010827
			WO 2003-JP6225	W	20030519

OTHER SOURCE(S): MARPAT 139:395802

GI



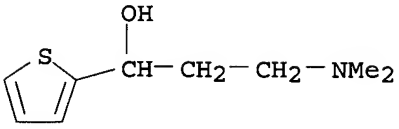
I

AB A process is provided, by which 3-N-methylamino-1-(2-thienyl)-1-propanols represented by the general formula (I)(wherein R1 is hydrogen, C1-8 acyl, substituted or unsubstituted C1-8 alkyloxycarbonyl, or substituted or unsubstituted phenyloxycarbonyl; and R2 is hydrogen, C1-8 alkyl, substituted or unsubstituted benzyl, C1-8 acyl, substituted or unsubstituted C1-8 alkyloxycarbonyl, or substituted or unsubstituted phenyloxycarbonyl, with the proviso that a case wherein R1 is hydrogen and R2 is Me or hydrogen is excepted) can be easily prepared in the form of a racemate or an optically active substance of S- or R-configuration at a low cost and in a high yield. The compds. I are useful as intermediates for drugs and agrochems., e.g. (S)-enantiomer for duloxetine (antidepressant). Thus, 36.9 g N-benzylmethylamine (0.30 mmol) was dissolved in 40 mL ethanol, treated with 30.0 g 37% aqueous HCl (0.30 mmol) to convert it to the hydrochloride salt, treated with 30 g 2-acetylthiophene, 10.8 g paraformaldehyde, 20 mL ethanol, and 1.2 g 37% aqueous HCl (0.01 mmol), heated at 80° under reflux for 4 h, cooled to room temperature, and filtered, followed by washing the crystals with ethanol and drying under reduced pressure to give 57.7 g 3-(N-benzylmethylamino)-1-(2-thienyl)-1-propanone (II) as the HCl salt. A 0.5 M KOH/2-propanol (40 μL), 2.1 mg (R,R)-1,2-diphenylethylenediamine, 873 mg II, and 3 mL 2-propanol were added to a Schlenk reaction tube, degassed and purged with Ar, treated with 9.6 mg RuCl2((R)-BINAP)(DMF)n, repeatedly degassed and purged with Ar, dissolved completely, transferred to a glass autoclave, pressurized with H, and stirred at 28° for 6 h to give (S)-3-(N-benzylmethylamino)-1-(2-thienyl)-1-propanol (96% ee).

IT 13636-02-7, 3-(Dimethylamino)-1-(2-thienyl)-1-propanol
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of (methylamino)thienylpropanols)

RN 13636-02-7 HCAPLUS

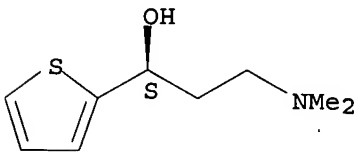
CN 2-Thiophenemethanol, α-[2-(dimethylamino)ethyl]- (CA INDEX NAME)



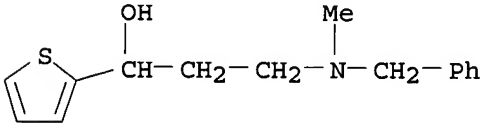
IT 132335-44-5P 138760-50-6P 625853-14-7P
625853-20-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (methylamino)thienylpropanols)

RN 132335-44-5 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(dimethylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

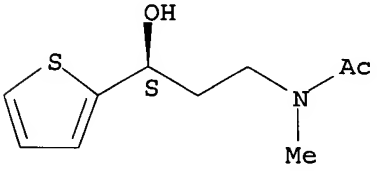


RN 138760-50-6 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[methyl(phenylmethyl)amino]ethyl]- (9CI) (CA INDEX NAME)



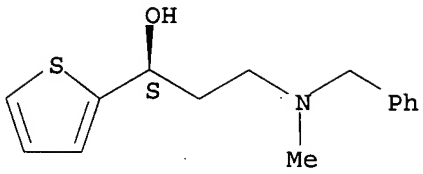
RN 625853-14-7 HCAPLUS
CN Acetamide, N-[(3S)-3-hydroxy-3-(2-thienyl)propyl]-N-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



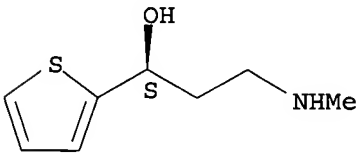
RN 625853-20-5 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[methyl(phenylmethyl)amino]ethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

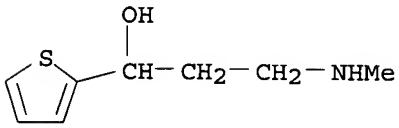


IT 116539-55-0P 116539-56-1P 625853-17-0P
625853-28-3P 625853-29-4P 625853-30-7P
625853-31-8P 625853-32-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of (methylamino)thienylpropanols)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

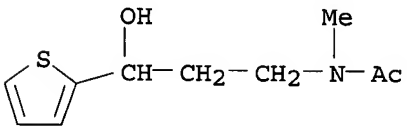
Absolute stereochemistry. Rotation (-).



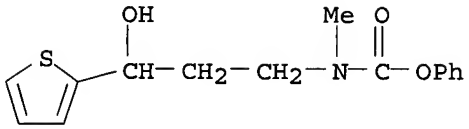
RN 116539-56-1 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]- (CA INDEX NAME)



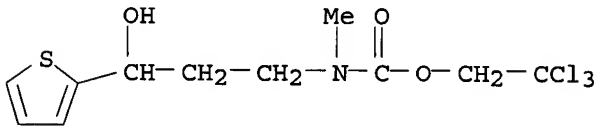
RN 625853-17-0 HCAPLUS
CN Acetamide, N-[3-hydroxy-3-(2-thienyl)propyl]-N-methyl- (9CI) (CA INDEX NAME)



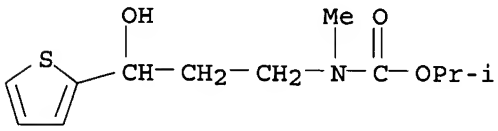
RN 625853-28-3 HCAPLUS
CN Carbamic acid, [3-hydroxy-3-(2-thienyl)propyl]methyl-, phenyl ester (9CI) (CA INDEX NAME)



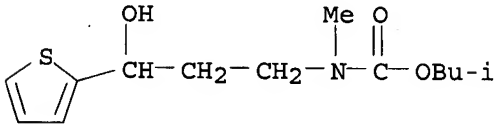
RN 625853-29-4 HCAPLUS
CN Carbamic acid, [3-hydroxy-3-(2-thienyl)propyl]methyl-, 2,2,2-trichloroethyl ester (9CI) (CA INDEX NAME)



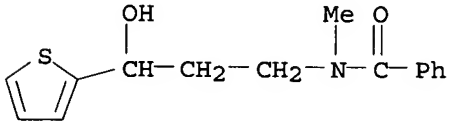
RN 625853-30-7 HCAPLUS
CN Carbamic acid, [3-hydroxy-3-(2-thienyl)propyl]methyl-, 1-methylethyl ester (9CI) (CA INDEX NAME)



RN 625853-31-8 HCAPLUS
CN Carbamic acid, [3-hydroxy-3-(2-thienyl)propyl]methyl-, 2-methylpropyl ester (9CI) (CA INDEX NAME)



RN 625853-32-9 HCAPLUS
CN Benzamide, N-[3-hydroxy-3-(2-thienyl)propyl]-N-methyl- (9CI) (CA INDEX NAME)



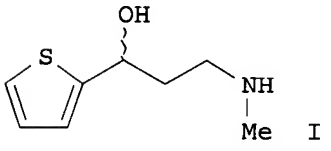
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN

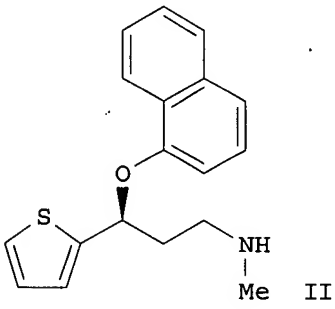
ACCESSION NUMBER: 2003:591163 HCAPLUS
DOCUMENT NUMBER: 139:149519
TITLE: Process for preparing (S)-3-methylamino-1-(2-thienyl)-1-propanol, an intermediate useful for the asymmetric synthesis of duloxetine, via optical resolution
INVENTOR(S): Borghese, Alfio
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 12 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2003062219	A1	20030731	WO 2003-US18		20030113
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
EP 1478641	A1	20041124	EP 2003-707289		20030113
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK					
US 2004249170	A1	20041209	US 2004-500829		20040707
PRIORITY APPLN. INFO.:			US 2002-351622P	P	20020124
			WO 2003-US18	W	20030113

GI



I



II

AB The invention provides an optical resolution process for the synthesis of (S)-3-methylamino-1-(2-thienyl)-1-propanol [(S)-I], a key intermediate in the synthesis of duloxetine (II) and its hydrochloride. The process comprises 3 distinct steps. The first step involves resolution of racemic I using either 2,3,4,6-di-O-isopropylidene-2-keto-L-gulonic acid (III) or (S)-(-)-2-pyrrolidone-5-carboxylic acid as the resolving agent, in a solvent which is preferably iso-PrOH, THF, acetone, or EtOAc, most preferably iso-PrOH. The second step involves racemization of a stereochem. enriched mixture, which may be the undesired isomer (R)-I,

and which may be carried out with HCl in iso-PrOH. The third step is a second order asym. induced crystallization of (S)-I, carried out by resolution of racemic I using III as the resolving agent, in a solvent as described above. For instance, a solution of racemic I in iso-PrOH was treated with III, stirred, and filtered to give the diastereomeric salt (S)-I.III in 74% yield and 12% d.e. (diastereomeric excess). Re-suspension of the product salt in iso-PrOH followed by stirring at room temperature and filtration (twice) increased the d.e. to 78% with losses in yield. In a demonstration of the racemization step, I.III with a d.e. of 75% was treated with 1N HCl for 2.5 h and concentrated in vacuo to give a solid showing a d.e. of 32%. In a demonstration of the 3rd step, racemic I and III in iso-PrOH were heated at 40° for 66 h and cooled and filtered to give crystalline (S)-I.III in 76% yield and 76% d.e. Mass balance anal. showed formation of the desired diastereomer at the expense of the unwanted one.

IT 569687-76-9P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(diastereomeric salt; process for preparation of a chiral duloxetine intermediate by optical resolution)

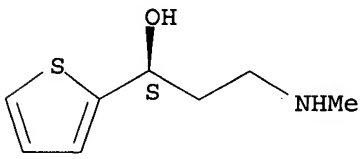
RN 569687-76-9 HCAPLUS

CN α-L-xylo-2-Hexulofuranosonic acid, 2,3:4,6-bis-O-(1-methylethylidene)-, compd. with (αS)-α-[2-(methylamino)ethyl]-2-thiophenemethanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 116539-55-0
CMF C8 H13 N O S

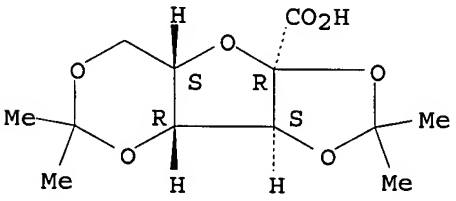
Absolute stereochemistry. Rotation (-).



CM 2

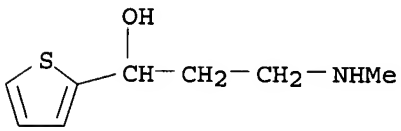
CRN 18467-77-1
CMF C12 H18 O7

Absolute stereochemistry. Rotation (-).



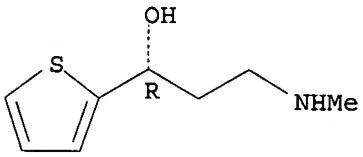
IT 116539-56-1, 3-Methylamino-1-(2-thienyl)-1-propanol
RL: RCT (Reactant); RACT (Reactant or reagent)

(racemic starting material; process for preparation of a chiral duloxetine intermediate by optical resolution)
RN 116539-56-1 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]- (CA INDEX NAME)



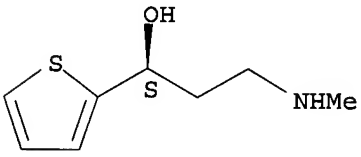
IT 116539-57-2P, (R)-3-Methylamino-1-(2-thienyl)-1-propanol
RL: BYP (Byproduct); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(racemization as undesired enantiomer; process for preparation of a chiral duloxetine intermediate by optical resolution)
RN 116539-57-2 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αR)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT 116539-55-0P, (S)-3-Methylamino-1-(2-thienyl)-1-propanol
RL: IMF (Industrial manufacture); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)
(target intermediate; process for preparation of a chiral duloxetine intermediate by optical resolution)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:405867 HCAPLUS
DOCUMENT NUMBER: 139:245838
TITLE: Chemoenzymatic synthesis of duloxetine and its enantiomer: lipase-catalyzed resolution of 3-hydroxy-3-(2-thienyl) propanenitrile

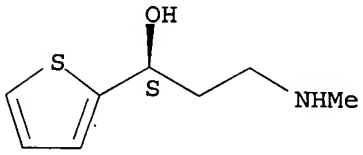
AUTHOR(S): Kamal, Ahmed; Khanna, G. B. Ramesh; Ramu, R.; Krishnaji, T.
CORPORATE SOURCE: Division of Organic Chemistry, Biotransformation Laboratory, Indian Institute of Chemical Technology, Hyderabad, 500 007, India
SOURCE: Tetrahedron Letters (2003), 44(25), 4783-4787
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:245838

AB An efficient and facile chemoenzymic synthesis of duloxetine by lipase-mediated resolution of 3-hydroxy-3-(2-thienyl)propanenitrile has been achieved. This process also describes an enantioconvergent synthesis of duloxetine via a Mitsunobu reaction.

IT 116539-55-0P 116539-57-2P 597581-29-8P
597581-30-1P 597581-31-2P
RL: BPN (Biosynthetic preparation); PUR (Purification or recovery); RCT (Reactant); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(chemoenzymic synthesis of duloxetine and its enantiomers via lipase-catalyzed resolution of hydroxy(thienyl)propanenitrile and its use in enantioconvergent synthesis of duloxetine via Mitsunobu reaction)

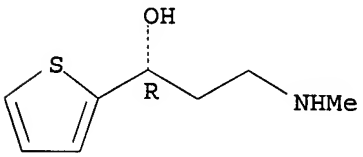
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



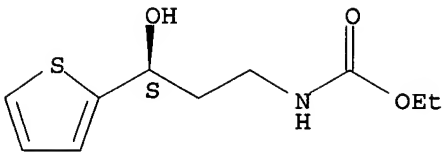
RN 116539-57-2 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αR)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



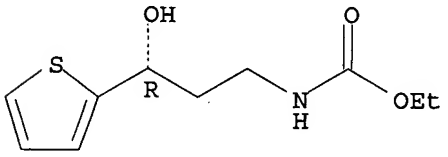
RN 597581-29-8 HCAPLUS
CN Carbamic acid, [(3S)-3-hydroxy-3-(2-thienyl)propyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



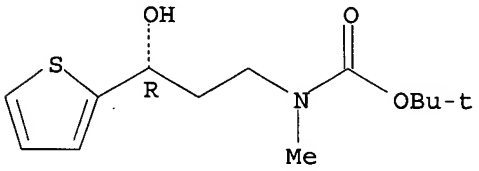
RN 597581-30-1 HCAPLUS
CN Carbamic acid, [(3R)-3-hydroxy-3-(2-thienyl)propyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 597581-31-2 HCAPLUS
CN Carbamic acid, [(3R)-3-hydroxy-3-(2-thienyl)propyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d l9 ibib abs hitstr tot

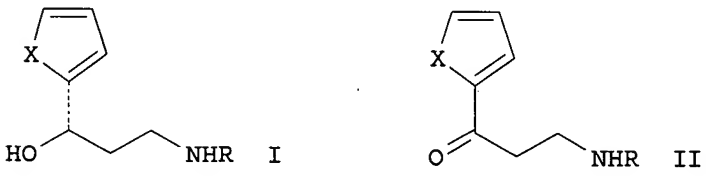
L9 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:181066 HCAPLUS
DOCUMENT NUMBER: 142:280046
TITLE: Process for the asymmetric hydrogenation of β-amino ketones using transition metal complexes of chiral bidentate phosphines as catalysts.
PATENT ASSIGNEE(S): Lonza AG, Switz.
SOURCE: Eur. Pat. Appl., 15 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

EP 1510517		A1	20050302	EP 2003-77734	20030901
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
AU 2004268057		A1	20050310	AU 2004-268057	20040831
WO 2005021527		A2	20050310	WO 2004-EP9690	20040831
WO 2005021527		A3	20050714		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1664014		A2	20060607	EP 2004-764655	20040831
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
CN 1842523		A	20061004	CN 2004-80024598	20040831
JP 2007504192		T	20070301	JP 2006-525092	20040831
NO 2006000763		A	20060317	NO 2006-763	20060217
US 2006252945		A1	20061109	US 2006-569824	20060228
PRIORITY APPLN. INFO.:				EP 2003-77734 A	20030901
				WO 2004-EP9690 W	20040831

OTHER SOURCE(S): CASREACT 142:280046; MARPAT 142:280046

GI



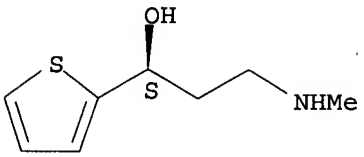
AB A process for the preparation of enantiomerically enriched or enantiomerically pure β-amino alcs. [I; X = S, O; R = (substituted) alkyl, cycloalkyl, aryl, aralkyl] comprises asym. hydrogenation of ketones (II; variables as above) using transition metal complexes of chiral bidentate phosphines as catalysts. Thus, 3-methylamino-1-(thien-2-yl)propan-1-one hydrochloride (preparation given), NaOMe, (S,S)-Me-DuPhos, and [Rh(COD)2]BF4 were autoclaved together in MeOH at 30-34° and 30 bar H2 for 5 h to give 67% (S)-3-methylamino-1-(2-thienyl)-1-propanol in >99% enantiomeric excess.

IT 116539-55-0P, (S)-3-Methylamino-1-(2-thienyl)-1-propanol
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(asym. hydrogenation of aminoketones using transition metal complexes of chiral bidentate phosphines as catalysts)

RN 116539-55-0 HCAPLUS

CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

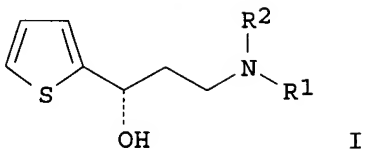


REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:101154 HCAPLUS
DOCUMENT NUMBER: 140:163699
TITLE: Process for the preparation of 3-hydroxy-(2-thienyl)propanamines by catalytic enantioselective hydrogenation of the corresponding ketones
INVENTOR(S): Hems, William; Rossen, Kai; Reichert, Dietmar; Koehler, Klaus; Almena Perea, Juan Jose
PATENT ASSIGNEE(S): Degussa A.-G., Germany
SOURCE: PCT Int. Appl., 27 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2004011452	A1	20040205	WO 2003-EP7927		20030721
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
DE 10233724	A1	20040205	DE 2002-10233724		20020724
DE 10258098	A1	20040701	DE 2002-10258098		20021211
CA 2493228	A1	20040205	CA 2003-2493228		20030721
AU 2003258532	A1	20040216	AU 2003-258532		20030721
EP 1523479	A1	20050420	EP 2003-771063		20030721
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK					
CN 1671685	A	20050921	CN 2003-817590		20030721
JP 2006502996	T	20060126	JP 2004-523756		20030721
US 2005272930	A1	20051208	US 2005-521799		20050121
IN 2005KN00259	A	20070105	IN 2005-KN259		20050224
PRIORITY APPLN. INFO.:			DE 2002-10233724	A	20020724
			DE 2002-10258098	A	20021211
			WO 2003-EP7927	W	20030721

OTHER SOURCE(S): CASREACT 140:163699; MARPAT 140:163699
GI



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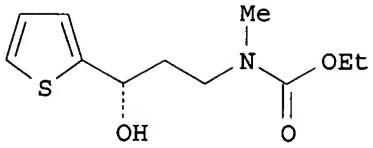


II

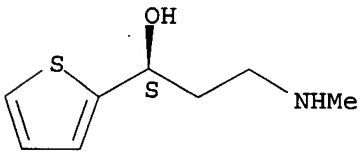
AB Title compds. I [wherein R1 and R2 = independently H, (cyclo)alkyl, acyl, alkoxycarbonyl, (hetero)aryl, (hetero)aralkyl, alkylcycloalkyl, alkyl(hetero)aryl; or NR1R2 = (un)substituted heterocyclyl], intermediates for the synthesis of enantiomer-pure bioactive substances, were prepared by catalytic enantioselective hydrogenation of the corresponding α-heteroaryl ketones. Inter alia Ru catalysts with chiral diamine and chiral biphosphine ligands were used. For example, 3-[N-ethoxycarbonyl-N-methylamino]-1-(2-thienyl)-1-propanone was introduced to a Buchi stirred autoclave, which was then evacuated. A mixture of (R)-TolBINAP-RuCl2-(1R,2R)-diphenylethylenediamine and KOBu-t in iPrOH was added. Flushing with H2, pressurizing to 10 bar, and heating to 40° for 2 h provided II in >96% yield with an enantiomeric excess of 80.1%. The content of cyclic carbamate byproduct increased significantly after standing for a fairly long time.

IT 116539-55-0P
RL: IMF (Industrial manufacture); PREP (Preparation)
(preparation of 3-hydroxy-(2-thienyl)propanamines by catalytic enantioselective hydrogenation of corresponding ketones)

RN 116539-55-0 HCAPLUS

CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

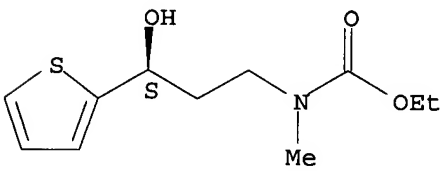


IT 586968-34-5P, (S)-3-[N-(Ethoxycarbonyl)-N-methylamino]-1-(2-thienyl)-1-propanol
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 3-hydroxy-(2-thienyl)propanamines by catalytic enantioselective hydrogenation of corresponding ketones)

RN 586968-34-5 HCAPLUS

CN Carbamic acid, [(3S)-3-hydroxy-3-(2-thienyl)propyl]methyl-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:757296 HCAPLUS
DOCUMENT NUMBER: 139:276809
TITLE: Process for preparing nonracemic chiral alcohols
INVENTOR(S): Tucker, Charles E.; Jiang, Qiongzhong
PATENT ASSIGNEE(S): DSM N.V., Neth.
SOURCE: U.S. Pat. Appl. Publ., 17 pp., Cont.-in-part of U.S.Ser.No. 57,826.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 7
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003181319	A1	20030925	US 2002-158560	20020521
US 2003144521	A1	20030731	US 2002-57826	20020124
US 6743921	B2	20040601		
WO 2003061826	A1	20030731	WO 2002-NL827	20021213

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2002-57826 A2 20020124
US 2002-158560 A 20020521

OTHER SOURCE(S): MARPAT 139:276809

AB The present invention provides a catalyst system and a process for the preparation of a nonracemic chiral alc. by hydrogenation of a ketone using the catalyst system, wherein the catalyst system comprises ruthenium, a nonracemic chiral diphosphine ligand, a bidentate amine ligand, and an organic base selected from alkylamidines, alkylguanidines, aminophosphazenes, and proazaphosphatranes. Thus, in a dry nitrogen-filled glovebox, a 20-mL glass reaction vial was charged with 5 mL 250 μL (1.25 μmol) [RuCl2(R,R,R,R-BICP)(DMF)n] (preparation given) in isopropanol, 5 mL isopropanol, and 125 μL 0.1 M (12.5 μmol) ethylenediamine in isopropanol. After stirring for several minutes, 73 μL (625 μmol) acetophenone was added, followed by 0.50 mL 0.1 M (50 μmol) tetramethyl-2-tert-butylguanidine in isopropanol. The glass reaction vial containing the resulting mixture was sealed in an autoclave and then removed from the glovebox. The gas phase in the autoclave was replaced by hydrogen at 18 bar and the reaction mixture was stirred at room temperature for 6 h under 17-18 bar hydrogen to give, after silica gel chromatog., (S)-1-phenylethanol (77% e.e.).

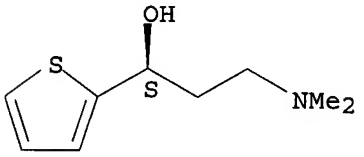
IT 132335-44-5P, (S)-3-(Dimethylamino)-1-(2-thienyl)-1-propanol
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of nonracemic chiral alcs. by stereoselective hydrogenation of ketone using catalyst system, comprising ruthenium complex,

nonracemic chiral diphosphine ligand, bidentate amine ligand, and organic base)

RN 132335-44-5 HCAPLUS

CN 2-Thiophenemethanol, α-[2-(dimethylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



=> d l12 ibib abs hitstr tot

L12 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:101154 HCAPLUS

DOCUMENT NUMBER: 140:163699

TITLE: Process for the preparation of 3-hydroxy-(2-thienyl)propanamines by catalytic enantioselective hydrogenation of the corresponding ketones

INVENTOR(S): Hems, William; Rossen, Kai; Reichert, Dietmar; Koehler, Klaus; Almena Perea, Juan Jose

PATENT ASSIGNEE(S): Degussa A.-G., Germany

SOURCE: PCT Int. Appl., 27 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

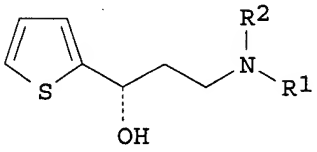
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004011452	A1	20040205	WO 2003-EP7927	20030721
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10233724	A1	20040205	DE 2002-10233724	20020724
DE 10258098	A1	20040701	DE 2002-10258098	20021211
CA 2493228	A1	20040205	CA 2003-2493228	20030721
AU 2003258532	A1	20040216	AU 2003-258532	20030721
EP 1523479	A1	20050420	EP 2003-771063	20030721
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1671685	A	20050921	CN 2003-817590	20030721
JP 2006502996	T	20060126	JP 2004-523756	20030721
US 2005272930	A1	20051208	US 2005-521799	20050121

IN 2005KN00259 A 20070105 IN 2005-KN259 20050224
PRIORITY APPLN. INFO.: DE 2002-10233724 A 20020724
DE 2002-10258098 A 20021211
WO 2003-EP7927 W 20030721
OTHER SOURCE(S): CASREACT 140:163699; MARPAT 140:163699
GI



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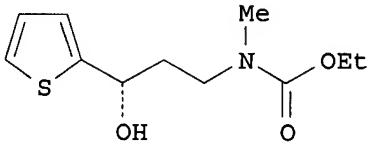


II

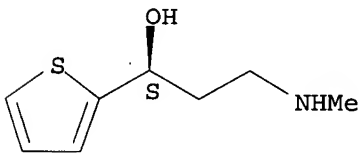
AB Title compds. I [wherein R1 and R2 = independently H, (cyclo)alkyl, acyl, alkoxycarbonyl, (hetero)aryl, (hetero)aralkyl, alkylcycloalkyl, alkyl(hetero)aryl; or NR1R2 = (un)substituted heterocyclyl], intermediates for the synthesis of enantiomer-pure bioactive substances, were prepared by catalytic enantioselective hydrogenation of the corresponding α-heteroaryl ketones. Inter alia Ru catalysts with chiral diamine and chiral biphosphine ligands were used. For example, 3-[N-ethoxycarbonyl-N-methylamino]-1-(2-thienyl)-1-propanone was introduced to a Buchi stirred autoclave, which was then evacuated. A mixture of (R)-TolBINAP-RuCl2-(1R,2R)-diphenylethylenediamine and KOBu-t in iPrOH was added. Flushing with H2, pressurizing to 10 bar, and heating to 40° for 2 h provided II in >96% yield with an enantiomeric excess of 80.1%. The content of cyclic carbamate byproduct increased significantly after standing for a fairly long time.

IT 116539-55-0P
RL: IMF (Industrial manufacture); PREP (Preparation)
(preparation of 3-hydroxy-(2-thienyl)propanamines by catalytic enantioselective hydrogenation of corresponding ketones)

RN 116539-55-0 HCAPLUS

CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

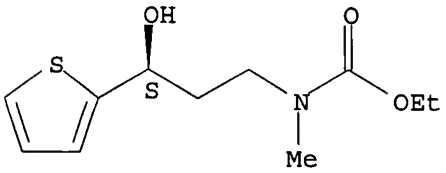


IT 586968-34-5P, (S)-3-[N-(Ethoxycarbonyl)-N-methylamino]-1-(2-thienyl)-1-propanol
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 3-hydroxy-(2-thienyl)propanamines by catalytic enantioselective hydrogenation of corresponding ketones)

RN 586968-34-5 HCAPLUS

CN Carbamic acid, [(3S)-3-hydroxy-3-(2-thienyl)propyl]methyl-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

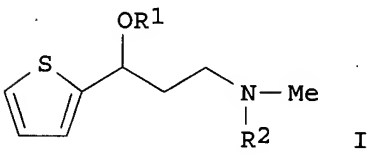


REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:931354 HCAPLUS
DOCUMENT NUMBER: 139:395802
TITLE: Preparation of propanolamine derivatives, process for preparation of 3-N-methylamino-1-(2-thienyl)-1-propanols, and process for preparation of propanolamine derivatives
INVENTOR(S): Inoue, Yoshiki; Mori, Hiroyuki; Nogami, Hiroyuki; Saitou, Takayuki; Ogura, Kuniyoshi
PATENT ASSIGNEE(S): Mitsubishi Rayon Co., Ltd., Japan
SOURCE: PCT Int. Appl., 98 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2003097632	A1	20031127	WO 2003-JP6225		20030519
W: CN, JP, US					
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR					
EP 1506965	A1	20050216	EP 2003-752916		20030519
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK					
US 2006167278	A1	20060727	US 2005-513790		20050527
PRIORITY APPLN. INFO.:			JP 2002-145394	A	20020520
			JP 2001-256621	A	20010827
			WO 2003-JP6225	W	20030519

OTHER SOURCE(S): MARPAT 139:395802
GI



I

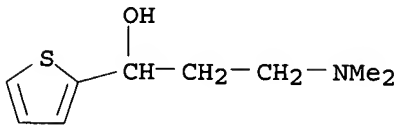
AB A process is provided, by which 3-N-methylamino-1-(2-thienyl)-1-propanols represented by the general formula (I)(wherein R1 is hydrogen, C1-8 acyl, substituted or unsubstituted C1-8 alkyloxycarbonyl, or substituted or unsubstituted phenyloxycarbonyl; and R2 is hydrogen, C1-8

alkyl, substituted or unsubstituted benzyl, C1-8 acyl, substituted or unsubstituted C1-8 alkyloxycarbonyl, or substituted or unsubstituted phenyloxycarbonyl, with the proviso that a case wherein R1 is hydrogen and R2 is Me or hydrogen is excepted) can be easily prepared in the form of a racemate or an optically active substance of S- or R-configuration at a low cost and in a high yield. The compds. I are useful as intermediates for drugs and agrochems., e.g. (S)-enantiomer for duloxetine (antidepressant). Thus, 36.9 g N-benzylmethylamine (0.30 mmol) was dissolved in 40 mL ethanol, treated with 30.0 g 37% aqueous HCl (0.30 mmol) to convert it to the hydrochloride salt, treated with 30 g 2-acetylthiophene, 10.8 g paraformaldehyde, 20 mL ethanol, and 1.2 g 37% aqueous HCl (0.01 mmol), heated at 80° under reflux for 4 h, cooled to room temperature, and filtered, followed by washing the crystals with ethanol and drying under reduced pressure to give 57.7 g 3-(N-benzylmethylamino)-1-(2-thienyl)-1-propanone (II) as the HCl salt. A 0.5 M KOH/2-propanol (40 μL), 2.1 mg (R,R)-1,2-diphenylethylenediamine, 873 mg II, and 3 mL 2-propanol were added to a Schlenk reaction tube, degassed and purged with Ar, treated with 9.6 mg RuCl2((R)-BINAP)(DMF)n, repeatedly degassed and purged with Ar, dissolved completely, transferred to a glass autoclave, pressurized with H, and stirred at 28° for 6 h to give (S)-3-(N-benzylmethylamino)-1-(2-thienyl)-1-propanol (96% ee).

IT 13636-02-7, 3-(Dimethylamino)-1-(2-thienyl)-1-propanol
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of (methylamino)thienylpropanols)

RN 13636-02-7 HCAPLUS

CN 2-Thiophenemethanol, α-[2-(dimethylamino)ethyl]- (CA INDEX NAME)

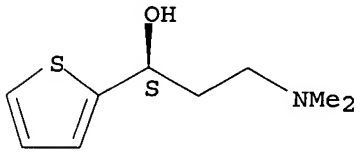


IT 132335-44-5P 138760-50-6P 625853-14-7P
625853-20-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (methylamino)thienylpropanols)

RN 132335-44-5 HCAPLUS

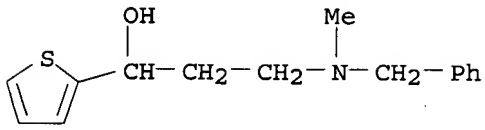
CN 2-Thiophenemethanol, α-[2-(dimethylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



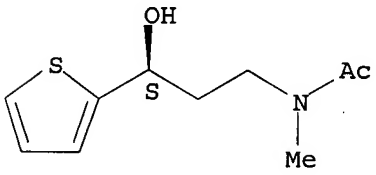
RN 138760-50-6 HCAPLUS

CN 2-Thiophenemethanol, α-[2-[methyl(phenylmethyl)amino]ethyl]- (9CI) (CA INDEX NAME)



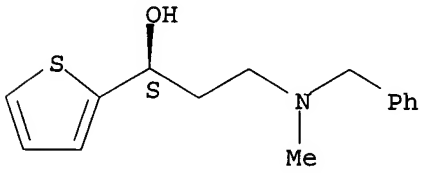
RN 625853-14-7 HCAPLUS
CN Acetamide, N-[(3S)-3-hydroxy-3-(2-thienyl)propyl]-N-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



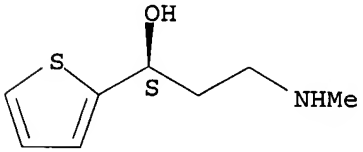
RN 625853-20-5 HCAPLUS
CN 2-Thiophenemethanol, α-[2-[methyl(phenylmethyl)amino]ethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

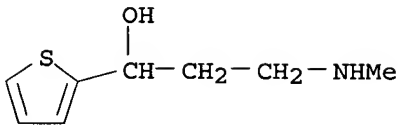


IT 116539-55-0P 116539-56-1P 625853-17-0P
625853-28-3P 625853-29-4P 625853-30-7P
625853-31-8P 625853-32-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of (methylamino)thienylpropanols)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

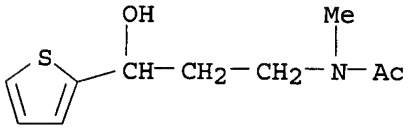
Absolute stereochemistry. Rotation (-).



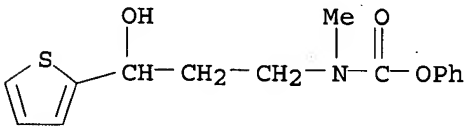
RN 116539-56-1 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]- (CA INDEX NAME)



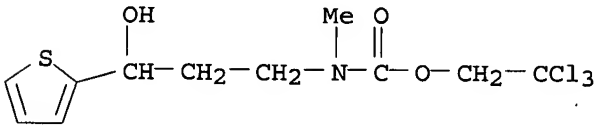
RN 625853-17-0 HCAPLUS
CN Acetamide, N-[3-hydroxy-3-(2-thienyl)propyl]-N-methyl- (9CI) (CA INDEX NAME)



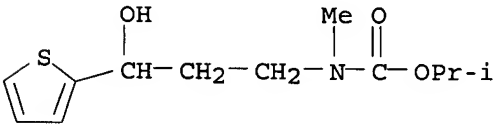
RN 625853-28-3 HCAPLUS
CN Carbamic acid, [3-hydroxy-3-(2-thienyl)propyl]methyl-, phenyl ester (9CI) (CA INDEX NAME)



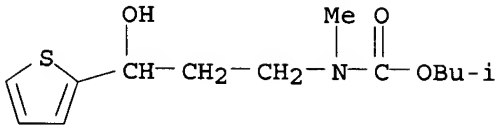
RN 625853-29-4 HCAPLUS
CN Carbamic acid, [3-hydroxy-3-(2-thienyl)propyl]methyl-, 2,2,2-trichloroethyl ester (9CI) (CA INDEX NAME)



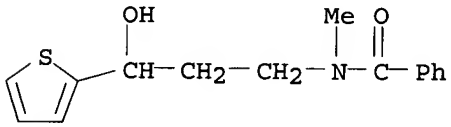
RN 625853-30-7 HCAPLUS
CN Carbamic acid, [3-hydroxy-3-(2-thienyl)propyl]methyl-, 1-methylethyl ester (9CI) (CA INDEX NAME)



RN 625853-31-8 HCAPLUS
CN Carbamic acid, [3-hydroxy-3-(2-thienyl)propyl]methyl-, 2-methylpropyl ester (9CI) (CA INDEX NAME)



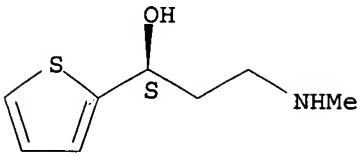
RN 625853-32-9 HCAPLUS
CN Benzamide, N-[3-hydroxy-3-(2-thienyl)propyl]-N-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

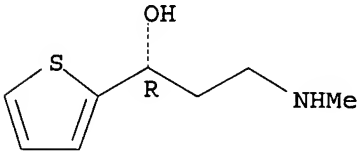
L12 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:405867 HCAPLUS
DOCUMENT NUMBER: 139:245838
TITLE: Chemoenzymatic synthesis of duloxetine and its enantiomer: lipase-catalyzed resolution of 3-hydroxy-3-(2-thienyl) propanenitrile
AUTHOR(S): Kamal, Ahmed; Khanna, G. B. Ramesh; Ramu, R.; Krishnaji, T.
CORPORATE SOURCE: Division of Organic Chemistry, Biotransformation Laboratory, Indian Institute of Chemical Technology, Hyderabad, 500 007, India
SOURCE: Tetrahedron Letters (2003), 44(25), 4783-4787
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:245838
AB An efficient and facile chemoenzymic synthesis of duloxetine by lipase-mediated resolution of 3-hydroxy-3-(2-thienyl)propanenitrile has been achieved. This process also describes an enantioconvergent synthesis of duloxetine via a Mitsunobu reaction.
IT 116539-55-0P 116539-57-2P 597581-29-8P
597581-30-1P 597581-31-2P
RL: BPN (Biosynthetic preparation); PUR (Purification or recovery); RCT (Reactant); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(chemoenzymic synthesis of duloxetine and its enantiomers via lipase-catalyzed resolution of hydroxy(thienyl)propanenitrile and its use in enantioconvergent synthesis of duloxetine via Mitsunobu reaction)
RN 116539-55-0 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



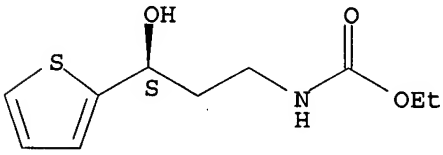
RN 116539-57-2 HCAPLUS
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αR)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



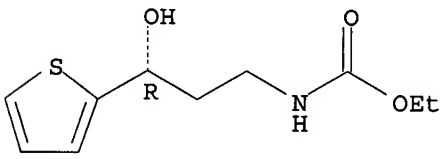
RN 597581-29-8 HCAPLUS
CN Carbamic acid, [(3S)-3-hydroxy-3-(2-thienyl)propyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



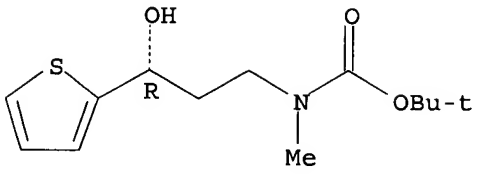
RN 597581-30-1 HCAPLUS
CN Carbamic acid, [(3R)-3-hydroxy-3-(2-thienyl)propyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 597581-31-2 HCAPLUS
CN Carbamic acid, [(3R)-3-hydroxy-3-(2-thienyl)propyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L8 ANSWER 1 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1251751 HCAPLUS
DOCUMENT NUMBER: 146:27718
TITLE: Etherification and resolution and demethylation process for the preparation of duloxetine and its acid-addition salts
INVENTOR(S): Satyanarayana, Chava; Ramanjaneyulu, Gorantla Seeta; Ramdas, Chavakula; Rao, Konudula Babu
PATENT ASSIGNEE(S): Matrix Laboratories Ltd, India
SOURCE: PCT Int. Appl., 18pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006126213	A1	20061130	WO 2006-IN174	20060523

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

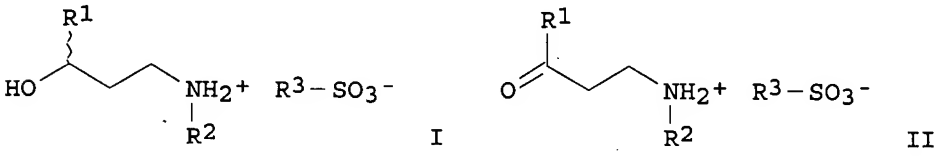
PRIORITY APPLN. INFO.: IN 2005-CH623 A 20050524
OTHER SOURCE(S): CASREACT 146:27718
AB A process for preparing duloxetine, or its acid addition salts (e.g., the hydrochloride), comprises: (A) the etherification of (S)-(-)-N,N-dimethyl-3-(2-thienyl)-3-hydroxypropanamine with 1-fluoronaphthalene, followed by demethylation, or etherification of N,N-dimethyl-3-(2-thienyl)-3-hydroxypropanamine with 1-fluoronaphthalene followed by resolution and demethylation; and (B) if desired, the neutralization of duloxetine free base into an acid-addition salt.
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:866581 HCAPLUS

DOCUMENT NUMBER: 145:271387
TITLE: Process for the preparation of enantiomerically pure 1-substituted-3-amino alcohols using methyl ketones, primary amines, formaldehydes and sulfonic acids
INVENTOR(S): Brieden, Walter; Clausen, Martin; McGarrity, John; Mettler, Hanspeter; Michel, Dominique
PATENT ASSIGNEE(S): Lonza A.-G., Switz.
SOURCE: PCT Int. Appl., 38pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006087166	A1	20060824	WO 2006-EP1334	20060214
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
EP 1693371	A1	20060823	EP 2005-3657	20050221
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, BA, HR, IS, YU				

PRIORITY APPLN. INFO.: EP 2005-3657 A 20050221
OTHER SOURCE(S): CASREACT 145:271387; MARPAT 145:271387
GI



AB Provided is a process for the preparation of N-monosubstituted β-aminoalc. sulfonates of formula I. Compds. of formula I wherein R1 is (un)substituted C6-20 aryl or (un)substituted C4-12 heteroaryl; R2 is C1-4-alkyl or (un)substituted C6-20 aryl; R3 is selected from the group consisting of C1-18 alkyl, C6-20 cycloalkyl, C6-20 aryl and C7-20 aralkyl residues, and the process for preparing compds. of formula I are claimed. The process comprising the steps of a) reacting a Me ketone, a primary amine, formaldehyde and a sulfonic acid, at a pressure above 1.5 bar, optionally in a organic solvent, said organic solvent optionally containing water, to afford N-monosubstituted β-amino ketone sulfonates of formula II, wherein R1, R2 and R3 are as defined above, and b) asym. hydrogenating said sulfonates in the presence of a base and a catalyst, comprising a transition metal and a diphosphine ligand,

in a polar solvent, optionally in the presence of water.
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

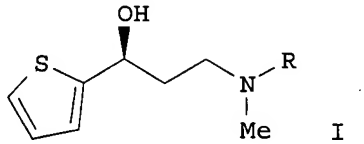
L8 ANSWER 3 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:985346 HCAPLUS
DOCUMENT NUMBER: 143:286275
TITLE: Process for the preparation of N-alkyl-N-methyl-3-hydroxy-3-(2-thienyl)-propylamines
INVENTOR(S): Schiffers, Robert; Kreye, Paul; Baumgarten, Wolfgang; Collet, Rosemarie
PATENT ASSIGNEE(S): Boehringer Ingelheim International GmbH, Germany
SOURCE: U.S. Pat. Appl. Publ., 7 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005197503	A1	20050908	US 2005-60510	20050216
DE 102004032828	A1	20060223	DE 2004-102004032828	20040706
CA 2556994	A1	20050915	CA 2005-2556994	20050226
WO 2005085192	A1	20050915	WO 2005-EP2047	20050226

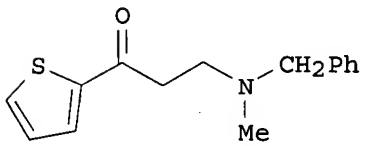
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:		
EP 2004-5272	A	20040305
DE 2004-102004032828	A	20040706
WO 2005-EP2047	W	20050226

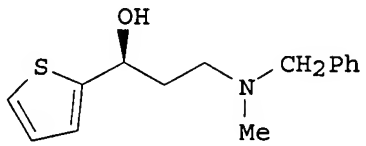
OTHER SOURCE(S): CASREACT 143:286275; MARPAT 143:286275
GI



I



II



III

AB An improved process for preparing chiral N-substituted N-methyl-3-hydroxy-3-(2-thienyl)-propylamines of formula I [R = C1-6 alkyl

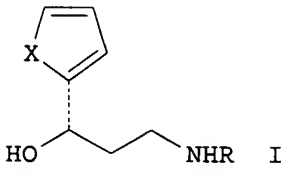
group optionally substituted by Ph, or an acid addition salt thereof] on an industrial scale is reported. An asym. hydrogenation using a catalyst system consisting of rhodium and (2R, 4R)-4-(dicyclohexylphosphino)-2-(diphenyl-phosphino-methyl)-N-methyl-aminocarbonyl-pyrrolidine is the key step. Thus II·HCl is hydrogenated at 40° C and 50 bar hydrogen pressure for about 20 h in the presence of bis-(1,5-cyclooctadiene)dirhodium(I)dichloride and (2R,4R)-4-(dicyclohexylphosphino)-2-(diphenyl-phosphino-methyl)-N-methyl-aminocarbonyl-pyrrolidine to provide III in 98% enantiomeric purity after workup.

L8 ANSWER 4 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:181066 HCAPLUS
DOCUMENT NUMBER: 142:280046
TITLE: Process for the asymmetric hydrogenation of β-amino ketones using transition metal complexes of chiral bidentate phosphines as catalysts.
PATENT ASSIGNEE(S): Lonza AG, Switz.
SOURCE: Eur. Pat. Appl., 15 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

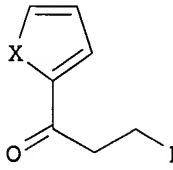
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1510517	A1	20050302	EP 2003-77734	20030901
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
AU 2004268057	A1	20050310	AU 2004-268057	20040831
WO 2005021527	A2	20050310	WO 2004-EP9690	20040831
WO 2005021527	A3	20050714		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1664014	A2	20060607	EP 2004-764655	20040831
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
CN 1842523	A	20061004	CN 2004-80024598	20040831
JP 2007504192	T	20070301	JP 2006-525092	20040831
NO 2006000763	A	20060317	NO 2006-763	20060217
US 2006252945	A1	20061109	US 2006-569824	20060228

PRIORITY APPLN. INFO.:	EP 2003-77734	A	20030901
	WO 2004-EP9690	W	20040831

OTHER SOURCE(S): CASREACT 142:280046; MARPAT 142:280046
GI



I



II

AB A process for the preparation of enantiomerically enriched or enantiomerically pure β-amino alcs. [I; X = S, O; R = (substituted) alkyl, cycloalkyl, aryl, aralkyl] comprises asym. hydrogenation of ketones (II; variables as above) using transition metal complexes of chiral bidentate phosphines as catalysts. Thus, 3-methylamino-1-(thien-2-yl)propan-1-one hydrochloride (preparation given), NaOMe, (S,S)-Me-DuPhos, and [Rh(COD)2]BF4 were autoclaved together in MeOH at 30-34° and 30 bar H2 for 5 h to give 67% (S)-3-methylamino-1-(2-thienyl)-1-propanol in >99% enantiomeric excess.

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 5 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:1037091 HCAPLUS
DOCUMENT NUMBER: 142:23180
TITLE: Process for producing optically active N-monoalkyl-3-hydroxy-3-arylpropylamine compound and intermediate
INVENTOR(S): Iwakura, Kazunori; Higashii, Takayuki; Bando, Seiji
PATENT ASSIGNEE(S): Sumitomo Seika Chemicals Co. Ltd., Japan
SOURCE: PCT Int. Appl., 35 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004103990	A1	20041202	WO 2004-JP6602	20040511
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP 2004346008	A	20041209	JP 2003-144742	20030522

PRIORITY APPLN. INFO.: JP 2003-144742 A 20030522
OTHER SOURCE(S): CASREACT 142:23180; MARPAT 142:23180

AB There is provided a process for producing an optically active N-monoalkyl-3-oxo-3-arylpropylamine compound represented by the formula ArC*H(OH)CH2CH2NHR1 (wherein symbol * indicates an asym. carbon atom; R1 represents optionally substituted C1-5 alkyl; Ar represents optionally substituted aryl or heteroaryl) characterized by asym. reducing a (Z)-protected-N-monoalkyl-3-oxo-3-arylpropenylamine compound represented by

the formula (Z)-ArCOCH:CHNR1R2 (wherein Ar and R1 are same as defined above; R2 represents an amino-protecting group) with an asym. catalyst to give an optically active compound represented by the formula ArC*H(OH)CH2CH2NR1R2 (wherein the symbol *, Ar, R1, and R2 are same as defined above) and successively eliminating the protective group (R2). Thus, 16.7 g (Z)-N-methyl-3-oxo-3-(2-thienyl)propenylamine was acylated by 16.4 g iso-Bu chlorocarbonate in the presence of 1.2 g 4-dimethylaminopyridine and 12.1 g Et3N in 200 mL tert-Bu Me ether at 50° for 28 h to give 22.0 g N-methyl-N-isobutoxycarbonyl-[(Z)-3-oxo-3-(2-thienyl)propenyl]amine (I). I (33.8 mg) was stirred in 2-propanol in the presence of potassium tert-butoxide and 2.3 mg [(S)-N-phenyl-2-azetidinecarboxamide]ruthenium(p-cymene) chloride (REG 543689-61-8) at 80° for 4 h to give 84% N-methyl-N-isobutoxycarbonyl-3-hydroxy-3-(2-thienyl)propylamine which (114.8 mg) was treated with a mixture of 0.2 g 30 weight% aqueous NaOH and 5 mL 2-propanol at 30° for 24 h to give N-methyl-3-hydroxy-3-(2-thienyl)propylamine (50% ee).

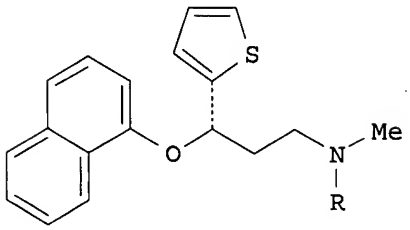
REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 6 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:546493 HCAPLUS
DOCUMENT NUMBER: 141:106360
TITLE: A process of preparation of (+)-duloxetine
INVENTOR(S): Rao, Dharmaraj Ramachandra; Kankan, Rajendra Narayanrao; Wain, Christopher Paul
PATENT ASSIGNEE(S): Cipla Ltd, India
SOURCE: PCT Int. Appl., 24 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004056795	A1	20040708	WO 2003-GB5357	20031210
WO 2004056795	A8	20050811		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2510750	A1	20040708	CA 2003-2510750	20031210
AU 2003292396	A1	20040714	AU 2003-292396	20031210
BR 2003016902	A	20051025	BR 2003-16902	20031210
EP 1587801	A1	20051026	EP 2003-767973	20031210
EP 1587801	B1	20070131		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1747947	A	20060315	CN 2003-80109793	20031210
JP 2006514030	T	20060427	JP 2004-561607	20031210
EP 1690861	A2	20060816	EP 2006-75798	20031210
EP 1690861	A3	20060906		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LV, FI, RO, CY, TR, BG, CZ, EE, HU, SK				

AT 353081	T	20070215	AT 2003-767973	20031210
IN 2005MN00657	A	20050930	IN 2005-MN657	20050623
US 2006205956	A1	20060914	US 2006-539415	20060320
PRIORITY APPLN. INFO.:			GB 2002-29583 A	20021219
			EP 2003-767973 A3	20031210
			WO 2003-GB5357 W	20031210

OTHER SOURCE(S): CASREACT 141:106360; MARPAT 141:106360
GI



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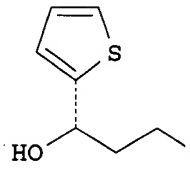


II

AB The invention relates to a process for preparing (+)-duloxetine (I), or an acid addition salt thereof, which comprises (a) resolving racemic (±)-duloxetine with a chiral acid so as to obtain a salt of the chiral acid and (+)-duloxetine, substantially free of (-)-duloxetine; and (b) if desired, converting the salt prepared in step (a) to the free base or another acid addition salt as appropriate. The process for preparing (+)-duloxetine, or an acid addition salt thereof, can further comprise an O-alkylation intermediate process step which is carried out in the presence of a base and a phase transfer catalyst. For instance, (S)-duloxetine hydrochloride (I•HCl, R = H) was prepared via etherification of alc. II by 1-fluoronaphthalene in the presence of 18-crown-6, and subsequent N-demethylation of the obtained oxalate salt of I (R = Me) (example 4 and 5).

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 7 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:120843 HCAPLUS
DOCUMENT NUMBER: 140:181317
TITLE: Preparation of enantiomerically pure (S)-3-methylamino-1-(thien-2-yl)propan-1-ol from racemic 3-hydroxy-3-(thien-2-yl)propionitrile via kinetic resolution with an acylating agent and a lipase followed by treatment with methylamine and hydrogen in the presence of a catalyst.
INVENTOR(S): Stuermer, Rainer
PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 31 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004013123	A1	20040212	WO 2003-EP8492	20030731

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,

GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,
TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

DE 10235206	A1	20040219	DE 2002-10235206		20020801
CA 2493451	A1	20040212	CA 2003-2493451		20030731
AU 2003251677	A1	20040223	AU 2003-251677		20030731
EP 1527065	A1	20050504	EP 2003-766383		20030731
EP 1527065	B1	20061122			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK					
CN 1671687	A	20050921	CN 2003-818510		20030731
JP 2006507234	T	20060302	JP 2004-525403		20030731
AT 346061	T	20061215	AT 2003-766383		20030731
US 2005245749	A1	20051103	US 2005-522888		20050624
PRIORITY APPLN. INFO.:			DE 2002-10235206	A	20020801
			WO 2003-EP8492	W	20030731

OTHER SOURCE(S): CASREACT 140:181317

AB A process for the preparation of enantiomerically pure (S)-3-methylamino-1-(thien-2-yl)propan-1-ol (I) comprises treatment of of a mixture of (R)- and (S)-3-hydroxy-3-thien-2-ylpropionitrile with an acylating agent in the presence of a hydrolase to give a mixture of unacylated (S)-3-hydroxy-3-thien-2-ylpropionitrile and acylated (R)-nitrile and treatment of the former with hydrogen and methylamine in the presence of a catalyst. Thus, 3-hydroxy-3-thien-2-ylpropionitrile (preparation given) was shaken with lipase from Pseudomonas DSM 8246 and vinyl hexanoate in Me tert-Bu ether for 6 h at room temperature to give after flash chromatog. 48% (S)-3-hydroxy-3-thien-2-ylpropionitrile in 99.4% enantiomeric excess. The latter was autoclaved with MeNH2 in MeOH over Raney Ni under 50 bar H2 at 65° for 24 h to give 79% I.

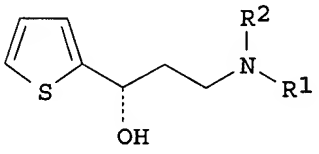
L8 ANSWER 8 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:101154 HCAPLUS
DOCUMENT NUMBER: 140:163699
TITLE: Process for the preparation of 3-hydroxy-(2-thienyl)propanamines by catalytic enantioselective hydrogenation of the corresponding ketones
INVENTOR(S): Hems, William; Rossen, Kai; Reichert, Dietmar; Koehler, Klaus; Almena Perea, Juan Jose
PATENT ASSIGNEE(S): Degussa A.-G., Germany
SOURCE: PCT Int. Appl., 27 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004011452	A1	20040205	WO 2003-EP7927	20030721
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,				

PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,
TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

DE 10233724	A1	20040205	DE 2002-10233724		20020724
DE 10258098	A1	20040701	DE 2002-10258098		20021211
CA 2493228	A1	20040205	CA 2003-2493228		20030721
AU 2003258532	A1	20040216	AU 2003-258532		20030721
EP 1523479	A1	20050420	EP 2003-771063		20030721
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK					
CN 1671685	A	20050921	CN 2003-817590		20030721
JP 2006502996	T	20060126	JP 2004-523756		20030721
US 2005272930	A1	20051208	US 2005-521799		20050121
IN 2005KN00259	A	20070105	IN 2005-KN259		20050224
PRIORITY APPLN. INFO.:			DE 2002-10233724	A	20020724
			DE 2002-10258098	A	20021211
			WO 2003-EP7927	W	20030721

OTHER SOURCE(S): CASREACT 140:163699; MARPAT 140:163699
GI



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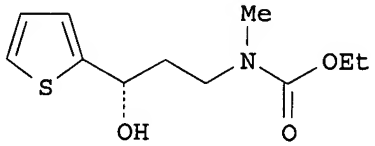


II

AB Title compds. I [wherein R1 and R2 = independently H, (cyclo)alkyl, acyl, alkoxycarbonyl, (hetero)aryl, (hetero)aralkyl, alkylcycloalkyl, alkyl(hetero)aryl; or NR1R2 = (un)substituted heterocyclyl], intermediates for the synthesis of enantiomer-pure bioactive substances, were prepared by catalytic enantioselective hydrogenation of the corresponding α-heteroaryl ketones. Inter alia Ru catalysts with chiral diamine and chiral biphosphine ligands were used. For example, 3-[N-ethoxycarbonyl-N-methylamino]-1-(2-thienyl)-1-propanone was introduced to a Buchi stirred autoclave, which was then evacuated. A mixture of (R)-TolBINAP-RuCl2-(1R,2R)-diphenylethylenediamine and KOBu-t in iPrOH was added. Flushing with H2, pressurizing to 10 bar, and heating to 40° for 2 h provided II in >96% yield with an enantiomeric excess of 80.1%. The content of cyclic carbamate byproduct increased significantly after standing for a fairly long time.

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

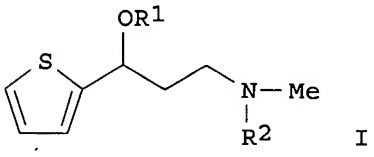
L8 ANSWER 9 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:931354 HCAPLUS
DOCUMENT NUMBER: 139:395802
TITLE: Preparation of propanolamine derivatives, process for preparation of 3-N-methylamino-1-(2-thienyl)-1-propanols, and process for preparation of propanolamine derivatives
INVENTOR(S): Inoue, Yoshiki; Mori, Hiroyuki; Nogami, Hiroyuki; Saitou, Takayuki; Ogura, Kuniyoshi
PATENT ASSIGNEE(S): Mitsubishi Rayon Co., Ltd., Japan

SOURCE: PCT Int. Appl., 98 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003097632	A1	20031127	WO 2003-JP6225	20030519
W: CN, JP, US				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				
EP 1506965	A1	20050216	EP 2003-752916	20030519
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2006167278	A1	20060727	US 2005-513790	20050527

PRIORITY APPLN. INFO.: JP 2002-145394 A 20020520
JP 2001-256621 A 20010827
WO 2003-JP6225 W 20030519

OTHER SOURCE(S): MARPAT 139:395802
GI



I

AB A process is provided, by which 3-N-methylamino-1-(2-thienyl)-1-propanols represented by the general formula (I)(wherein R1 is hydrogen, C1-8 acyl, substituted or unsubstituted C1-8 alkyloxycarbonyl, or substituted or unsubstituted phenyloxycarbonyl; and R2 is hydrogen, C1-8 alkyl, substituted or unsubstituted benzyl, C1-8 acyl, substituted or unsubstituted C1-8 alkyloxycarbonyl, or substituted or unsubstituted phenyloxycarbonyl, with the proviso that a case wherein R1 is hydrogen and R2 is Me or hydrogen is excepted) can be easily prepared in the form of a racemate or an optically active substance of S- or R-configuration at a low cost and in a high yield. The compds. I are useful as intermediates for drugs and agrochems., e.g. (S)-enantiomer for duloxetine (antidepressant). Thus, 36.9 g N-benzylmethylamine (0.30 mmol) was dissolved in 40 mL ethanol, treated with 30.0 g 37% aqueous HCl (0.30 mmol) to convert it to the hydrochloride salt, treated with 30 g 2-acetylthiophene, 10.8 g paraformaldehyde, 20 mL ethanol, and 1.2 g 37% aqueous HCl (0.01 mmol), heated at 80° under reflux for 4 h, cooled to room temperature, and filtered, followed by washing the crystals with ethanol and drying under reduced pressure to give 57.7 g 3-(N-benzylmethylamino)-1-(2-thienyl)-1-propanone (II) as the HCl salt. A 0.5 M KOH/2-propanol (40 μL), 2.1 mg (R,R)-1,2-diphenylethylenediamine, 873 mg II, and 3 mL 2-propanol were added to a Schlenk reaction tube, degassed and purged with Ar, treated with 9.6 mg RuCl2((R)-BINAP)(DMF)n, repeatedly degassed and purged with Ar, dissolved completely, transferred to a glass autoclave, pressurized with H, and stirred at 28° for 6 h to give (S)-3-(N-benzylmethylamino)-1-(2-thienyl)-1-propanol (96% ee).

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 10 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:757695 HCAPLUS
DOCUMENT NUMBER: 139:261165
TITLE: Process for preparation of 3-hydroxy-3-(2-thienyl)propionamide derivatives
INVENTOR(S): Takehara, Jun; Qu, Jingping; Kanno, Kazuaki; Kawabata, Hiroshi; Dekishima, Yasumasa; Ueda, Makoto; Endo, Kyoko; Murakami, Takeshi; Sasaki, Tomoko; Uehara, Hisatoshi; Matsumoto, Youichi; Suzuki, Shihomi
PATENT ASSIGNEE(S): Mitsubishi Chemical Corporation, Japan
SOURCE: PCT Int. Appl., 102 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003078418	A1	20030925	WO 2003-JP3170	20030317
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP 2003335732	A	20031128	JP 2002-141145	20020516
JP 2004067559	A	20040304	JP 2002-227401	20020805
JP 2004067560	A	20040304	JP 2002-227402	20020805
JP 2004067577	A	20040304	JP 2002-228495	20020806
JP 2003342275	A	20031203	JP 2002-317857	20021031
AU 2003221028	A1	20030929	AU 2003-221028	20030317
EP 1486493	A1	20041215	EP 2003-712723	20030317
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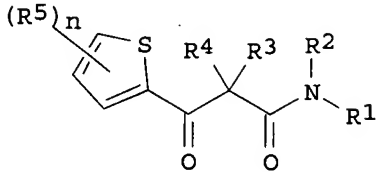
JP 2004155756	A	20040603	JP 2003-102914	20030407
US 2005107621	A1	20050519	US 2004-944055	20040920

PRIORITY APPLN. INFO.:

JP 2002-76168	A	20020319
JP 2002-129140	A	20020430
JP 2002-141145	A	20020516
JP 2002-227401	A	20020805
JP 2002-227402	A	20020805
JP 2002-228495	A	20020806
JP 2002-267617	A	20020913
JP 2002-317857	A	20021031
WO 2003-JP3170	W	20030317

OTHER SOURCE(S): MARPAT 139:261165
GI



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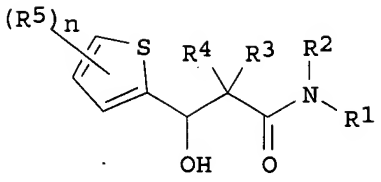

II

AB This invention pertains to a method for producing 3-oxo-3-(2-thienyl)propionamides with general formula of I [wherein R1 and R2 = independently H, alkyl, aryl, or aralkyl; R3 and R4 = independently H or alkyl; or R3 and R4 together form a ring with the nitrogen atom attached; R5 = halo, NO2, OH, (un)substituted alkyl, aryl, or alkoxy; n = 0-3] and a process for industrially producing optically active 3-amino-1-(2-thienyl)-1-propanol derivs. with general formula of II at low cost from the propionamides in high yields with high optical purity. The process comprises subjecting a β-ketocarbonyl compound having a thiophene ring to asym. reduction either in the presence of a catalyst comprising a compound of a Group 8 or 9 metal of the Periodic Table (e.g., ruthenium compound) and an asym. ligand (e.g., diphenylethylenediamine derivative) or using cells of a microorganism. Thus, 2-acetylthiophene was treated with NaH in THF, followed by the addition of di-Et carbonate to give 3-oxo-3-(2-thienyl)propionic acid Et ester (74%). The ester was treated with HCO2H in DMF in the presence of SS-TsDPEN and Et3N to provide (S)-3-hydroxy-3-(2-thienyl)propionic acid Et ester (94%) with 97.5% e.e. The chiral ester was treated with MeNH2 in MeOH to afford (S)-3-hydroxy-N-methyl-3-(2-thienyl)propionamide (93%) with 99% e.e.

REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 11 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:757296 HCAPLUS
DOCUMENT NUMBER: 139:276809
TITLE: Process for preparing nonracemic chiral alcohols
INVENTOR(S): Tucker, Charles E.; Jiang, Qiongzhong
PATENT ASSIGNEE(S): DSM N.V., Neth.
SOURCE: U.S. Pat. Appl. Publ., 17 pp., Cont.-in-part of U.S.Ser.No. 57,826.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 7
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003181319	A1	20030925	US 2002-158560	20020521
US 2003144521	A1	20030731	US 2002-57826	20020124
US 6743921	B2	20040601		
WO 2003061826	A1	20030731	WO 2002-NL827	20021213

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,

KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2002-57826 A2 20020124
US 2002-158560 A 20020521

OTHER SOURCE(S): MARPAT 139:276809

AB The present invention provides a catalyst system and a process for the preparation of a nonracemic chiral alc. by hydrogenation of a ketone using the catalyst system, wherein the catalyst system comprises ruthenium, a nonracemic chiral diphosphine ligand, a bidentate amine ligand, and an organic base selected from alkylamidines, alkylguanidines, aminophosphazenes, and proazaphosphatranes. Thus, in a dry nitrogen-filled glovebox, a 20-mL glass reaction vial was charged with 5 mL 250 μL (1.25 μmol) [RuCl2(R,R,R,R-BICP)(DMF)n] (preparation given) in isopropanol, 5 mL isopropanol, and 125 μL 0.1 M (12.5 μmol) ethylenediamine in isopropanol. After stirring for several minutes, 73 μL (625 μmol) acetophenone was added, followed by 0.50 mL 0.1 M (50 μmol) tetramethyl-2-tert-butylguanidine in isopropanol. The glass reaction vial containing the resulting mixture was sealed in an autoclave and then removed from the glovebox. The gas phase in the autoclave was replaced by hydrogen at 18 bar and the reaction mixture was stirred at room temperature for 6 h under 17-18 bar hydrogen to give, after silica gel chromatog., (S)-1-phenylethanol (77% e.e.).

L8 ANSWER 12 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:591066 HCAPLUS
DOCUMENT NUMBER: 139:151397
TITLE: Process for preparing nonracemic chiral alcohols by hydrogenation of ketones using ruthenium-based catalysts
INVENTOR(S): Tucker, Charles Edward; Jiang, Qiongzhong
PATENT ASSIGNEE(S): Dsm N.V., Neth.
SOURCE: PCT Int. Appl., 48 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 7
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003061825	A1	20030731	WO 2002-NL826	20021213
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003144521	A1	20030731	US 2002-57826	20020124
US 6743921	B2	20040601		
US 2003181318	A1	20030925	US 2002-158559	20020521

PRIORITY APPLN. INFO.: US 2002-57826 A 20020124
US 2002-158559 A 20020521

OTHER SOURCE(S): MARPAT 139:151397

AB The present invention provides a catalyst system and a process for the preparation of a nonracemic chiral alc. by hydrogenation of a ketone using the catalyst system, wherein the catalyst system comprises ruthenium, a nonracemic nonatropisomeric chiral diphosphine ligand, an achiral diamine ligand, and a base. Acetophenone was hydrogenated to S-1-phenethanol using a catalyst system containing RuCl2(benzene)2, (R,R,R,R)-2,2'-bis-(diphenylphosphino)-1,1'-dicyclopentane, 4,5-dimethyl-1,2-phenylenediamine, and sodium isopropoxide.

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 13 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:405867 HCAPLUS
DOCUMENT NUMBER: 139:245838
TITLE: Chemoenzymatic synthesis of duloxetine and its enantiomer: lipase-catalyzed resolution of 3-hydroxy-3-(2-thienyl) propanenitrile
AUTHOR(S): Kamal, Ahmed; Khanna, G. B. Ramesh; Ramu, R.; Krishnaji, T.
CORPORATE SOURCE: Division of Organic Chemistry, Biotransformation Laboratory, Indian Institute of Chemical Technology, Hyderabad, 500 007, India
SOURCE: Tetrahedron Letters (2003), 44(25), 4783-4787
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:245838

AB An efficient and facile chemoenzymic synthesis of duloxetine by lipase-mediated resolution of 3-hydroxy-3-(2-thienyl)propanenitrile has been achieved. This process also describes an enantioconvergent synthesis of duloxetine via a Mitsunobu reaction.

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 14 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:356091 HCAPLUS
DOCUMENT NUMBER: 138:353733
TITLE: Process for producing optically active amino alcohols
INVENTOR(S): Watanabe, Masahito; Murata, Kunihiko; Ikariya, Takao
PATENT ASSIGNEE(S): Kanto Kagaku Kabushiki Kaisha, Japan
SOURCE: Eur. Pat. Appl., 23 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1308435	A2	20030507	EP 2002-24517	20021030
EP 1308435	A3	20030604		
EP 1308435	B1	20051228		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
JP 2003201269	A	20030718	JP 2002-251994	20020829
JP 3504254	B2	20040308		
CA 2409906	A1	20030430	CA 2002-2409906	20021028

JP 2003201270	A	20030718	JP 2002-316217	20021030
US 2003171592	A1	20030911	US 2002-285164	20021031
US 6686505	B2	20040203		

PRIORITY APPLN. INFO.: JP 2001-335322 A 20011031
JP 2002-251994 A 20020829

OTHER SOURCE(S): MARPAT 138:353733

AB A process for producing an optically active amino alc. is provided that includes a step in which a nitro ketone or a cyano ketone is reacted with a hydrogen-donating organic or inorg. compound in the presence of a transition metal compound catalyst having an optically active nitrogen-containing compound as an asym. ligand to give an optically active nitro alc. or an optically active cyano alc., and a step in which the above optically active alc. is further reduced to efficiently produce an optically active amino alc. Thus, PhCOCH2CN was reduced with HCO2H in presence of Et3N and chloro[(S,S)-N-(p-toluenesulfonyl)-1,2-diphenylethylenediamine](p-cymene)ruthenium to give (S)-HOCHPhCH2CN in 98% ee. This compound was reduced with BH3.Me2S to give (S)-HOCHPhCH2CH2NH2 with 98% ee. The alcs. are intermediates for pharmaceuticals, such as fluoxetine, tomoxetine, nisoxetine and norfluoxetine.

L8 ANSWER 15 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:173596 HCAPLUS
DOCUMENT NUMBER: 138:221463
TITLE: Process for preparation of 3-(N-alkoxycarbonyl-N-methyl)amino-2-thienylpropan-1-ol derivatives
INVENTOR(S): Ikunaka, Masaya; Matsumoto, Jun; Inoue, Toru
PATENT ASSIGNEE(S): Nagase and Co., Ltd., Japan
SOURCE: PCT Int. Appl., 51 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003018572	A1	20030306	WO 2002-JP8588	20020826
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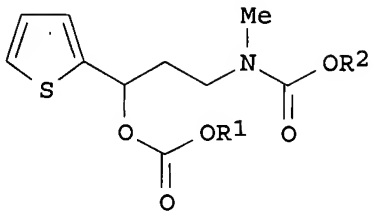
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP 2005053781	A	20050303	JP 2001-256621	20010827

PRIORITY APPLN. INFO.: JP 2001-256621 A 20010827
OTHER SOURCE(S): MARPAT 138:221463
GI



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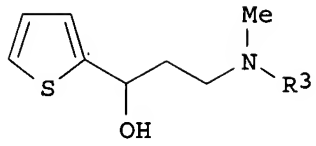

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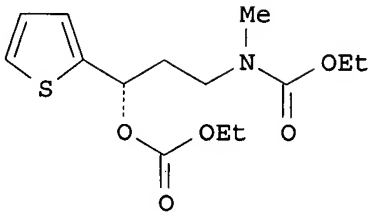

III

AB This invention pertains to prepn method of novel optically active 3-amino-2-thienylpropan-1-ol derivs. with general formula of I and II [wherein R1 and R2 = independently (un)substituted alkyl, alkoxy, alkenyl, alkynyl, (hetero)aralkyl, or (hetero)aryl; R3 = H or CO2R2]. Reaction of optically active 3-(N,N-dimethylamino)-1-(2-thienyl)propan-1-ol with a haloformic ester in the presence of a base provides I. Hydrolysis of I affords alc. II. For example, (S)-3-(N,N-dimethylamino)-1-(2-thienyl)propan-1-ol (96.2% e.e.) was treated with Et chloroformate in PhMe in the presence of NaHCO3 to give III (89%). Compound III was hydrolyzed with NaOH in EtOH and H2O to afford (S)-(2-thienyl)CH(OH)CH2CH2NHMe (80%) with 95.8% e.e.

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> FIL REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	136.75	310.86

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-19.50	-19.50

FILE 'REGISTRY' ENTERED AT 07:29:10 ON 15 APR 2007
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 13 APR 2007 HIGHEST RN 930268-90-9
DICTIONARY FILE UPDATES: 13 APR 2007 HIGHEST RN 930268-90-9

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TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

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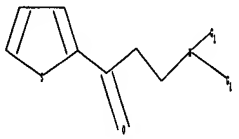

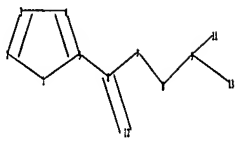

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6 7 8 9 11 12 13
ring nodes :
1 2 3 4 5
chain bonds :
5-6 6-7 6-12 7-8 8-9 9-11 9-13
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 6-12 8-9 9-11 9-13
exact bonds :
5-6 6-7 7-8

G1:H,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
11:CLASS 12:CLASS 13:CLASS

L13 STRUCTURE UPLOADED

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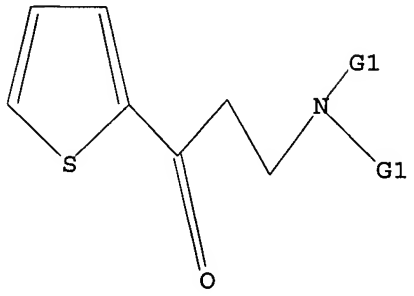
L13 HAS NO ANSWERS
L13 STR



G1 H,Ak

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED - 242 TO ITERATE

100.0% PROCESSED 242 ITERATIONS 30 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 3907 TO 5773
PROJECTED ANSWERS: 272 TO 928

L14 30 SEA SSS SAM L13

=> s l13 sss full
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FULL SCREEN SEARCH COMPLETED - 5232 TO ITERATE

100.0% PROCESSED 5232 ITERATIONS 494 ANSWERS
SEARCH TIME: 00.00.01

L15 494 SEA SSS FUL L13

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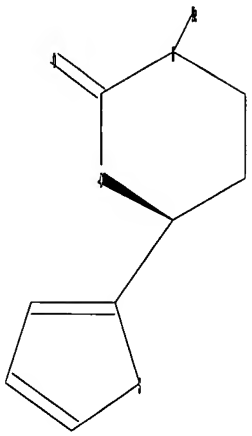

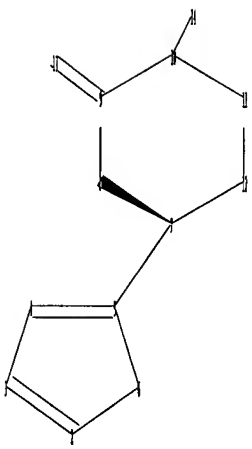

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ring nodes :
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chain bonds :
5-7 9-13 10-14
ring bonds :
2-3 2-6 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
7-8 7-12 8-9 9-10 9-13 10-11 11-12
exact bonds :
2-3 2-6 3-4 4-5 5-6 5-7 10-14
isolated ring systems :
containing 2 : 7 :

G1:H,Ak

Match level :
2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:Atom
12:Atom 13:CLASS 14:CLASS

Stereo Bonds:

8-7 (Single Wedge).

Stereo Chiral Centers:

7 (Parity=Don't Care)

Stereo RSS Sets:

Type=Relative (Default). 1 Nodes= 7

L16 STRUCTURE UPLOADED

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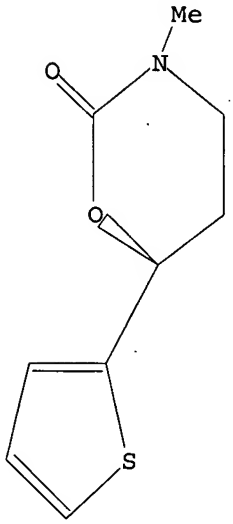
L16 HAS NO ANSWERS
L16 STR



G1 H,Ak

Structure attributes must be viewed using STN Express query preparation.

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                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:            2 TO      124
PROJECTED ANSWERS:               0 TO        0

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=> s l16 sss full
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FULL SCREEN SEARCH COMPLETED -       37 TO ITERATE

100.0% PROCESSED        37 ITERATIONS                             1 ANSWERS
SEARCH TIME: 00.00.01

L18             1 SEA SSS FUL L16

=> FIL HCAPLUS
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                                                      ENTRY    SESSION
FULL ESTIMATED COST                                  347.35     658.21

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
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CA SUBSCRIBER PRICE                                    0.00     -19.50

FILE 'HCAPLUS' ENTERED AT 07:34:50 ON 15 APR 2007
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FILE COVERS 1907 - 15 Apr 2007 VOL 146 ISS 17
FILE LAST UPDATED: 13 Apr 2007 (20070413/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L19 1 L18

=> d l19 ibib abs hitstr tot

L19 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:101154 HCAPLUS
DOCUMENT NUMBER: 140:163699
TITLE: Process for the preparation of 3-hydroxy-(2-thienyl)propanamines by catalytic enantioselective hydrogenation of the corresponding ketones
INVENTOR(S): Hems, William; Rossen, Kai; Reichert, Dietmar; Koehler, Klaus; Almena Perea, Juan Jose
PATENT ASSIGNEE(S): Degussa A.-G., Germany
SOURCE: PCT Int. Appl., 27 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004011452	A1	20040205	WO 2003-EP7927	20030721
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10233724	A1	20040205	DE 2002-10233724	20020724
DE 10258098	A1	20040701	DE 2002-10258098	20021211
CA 2493228	A1	20040205	CA 2003-2493228	20030721

AU 2003258532	A1	20040216	AU 2003-258532		20030721
EP 1523479	A1	20050420	EP 2003-771063		20030721
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK					
CN 1671685	A	20050921	CN 2003-817590		20030721
JP 2006502996	T	20060126	JP 2004-523756		20030721
US 2005272930	A1	20051208	US 2005-521799		20050121
IN 2005KN00259	A	20070105	IN 2005-KN259		20050224
PRIORITY APPLN. INFO.:			DE 2002-10233724	A	20020724
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			WO 2003-EP7927	W	20030721

OTHER SOURCE(S): CASREACT 140:163699; MARPAT 140:163699

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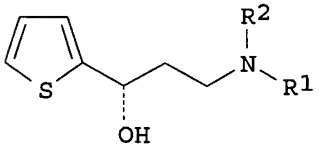

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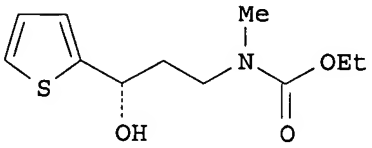


II

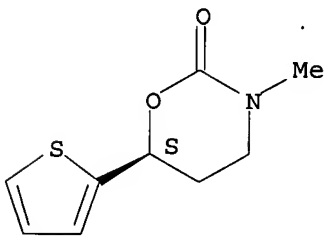
AB Title compds. I [wherein R1 and R2 = independently H, (cyclo)alkyl, acyl, alkoxycarbonyl, (hetero)aryl, (hetero)aralkyl, alkylcycloalkyl, alkyl(hetero)aryl; or NR1R2 = (un)substituted heterocyclyl], intermediates for the synthesis of enantiomer-pure bioactive substances, were prepared by catalytic enantioselective hydrogenation of the corresponding α-heteroaryl ketones. Inter alia Ru catalysts with chiral diamine and chiral biphosphine ligands were used. For example, 3-[N-ethoxycarbonyl-N-methylamino]-1-(2-thienyl)-1-propanone was introduced to a Buchi stirred autoclave, which was then evacuated. A mixture of (R)-TolBINAP-RuCl2-(1R,2R)-diphenylethylenediamine and KOBu-t in iPrOH was added. Flushing with H2, pressurizing to 10 bar, and heating to 40° for 2 h provided II in >96% yield with an enantiomeric excess of 80.1%. The content of cyclic carbamate byproduct increased significantly after standing for a fairly long time.

IT 654062-24-5P, (S)-3-Methyl-6-(2-thienyl)tetrahydro-2H-1,3-oxazin-2-one
RL: BYP (Byproduct); IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(cyclic carbamate; preparation of 3-hydroxy-(2-thienyl)propanamines by catalytic enantioselective hydrogenation of corresponding ketones)

RN 654062-24-5 HCAPLUS

CN 2H-1,3-Oxazin-2-one, tetrahydro-3-methyl-6-(2-thienyl)-, (6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	10.47	668.68

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.78	-20.28

STN INTERNATIONAL LOGOFF AT 07:35:46 ON 15 APR 2007